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Symmetry-preserving upwind discretization of convection on non-uniform grids

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Abstract

Although upwind discretization of convection will lead to a diagonally dominant coefficient matrix, on arbitrary grids the latter is not necessarily positive real, i.e. its symmetric part need not be positive definite ('negative diffusion'). Especially on contracting-expanding grids this property can be lost. The paper discusses a conservative (finite-volume) upwind variant for which the latter property is guaranteed to hold, irrespective of grid (ir)regularity. Further, empirically it is found that often its global discretization error is smaller than that of the 'traditional' (finite-difference) upwind method. Finally, it is shown that in many situations its extremal eigenvalues at the outer side of the spectrum move towards the imaginary axis, thus enhancing the stability of explicit time-integration methods.

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1. Introduction

Various flow problems in engineering practice are highly momentum driven, such as the wave impact phenomena studied in [8]. In such flows viscosity plays no physical role and there is no necessity to resolve thin viscous layers (often this is not even possible for an affordable price). What is required are efficient discretization schemes that keep the influence of the lack of viscous resolution to a minimum; asymptotic error behavior for vanishing grid size is only of secondary interest. Also, any contribution to better numerical handling (e.g. increased stability) is welcome.

The fact that viscosity is not relevant gives some algorithmic maneuvering space, as adding numerical viscosity will not immediately destroy the quality of the simulations. Thus for these applications, upwind discretization of the convective derivative can play the role as just described. It usually has a 'quiescent' influence on the discrete flow solutions by adding artificial diffusion to the problem. However, Golub et al. [1] have shown that on non-uniform grids this artificial diffusion can be of negative sign, in which case it can worsen the properties of the discretization.

In mathematical terms, although first-order upwind discretization leads to a diagonally-dominant matrix, it cannot guarantee that the coefficient matrix is positive real [32], i.e. its symmetric part need not be positive definite. This is

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a desirable property since it relates to the stability of the discrete solution, as can be understood from the following unsteady semi-discretized problem

$$\frac{d\phi_h}{dt} + L\phi_h = 0. \quad (1)$$

The discrete ‘energy’ of the solution given by $\|\phi_h\|_h^2 = \phi_h^* H \phi_h$, where the diagonal matrix H represents the local grid size, evolves in time according to

$$\frac{d}{dt} \|\phi_h\|_h^2 = \frac{d\phi_h^*}{dt} H \phi_h + \phi_h^* H \frac{d\phi_h}{dt} = -(L\phi_h)^* H \phi_h - \phi_h^* H L \phi_h = -\phi_h^* ((HL)^* + HL) \phi_h.$$

Hence the solution of (1) conserves energy if and only if the scaled coefficient matrix HL is skew symmetric. Furthermore, the energy is decreasing if and only if HL is positive real.

This observation has inspired many authors to design generalizations of second-order central discretization methods for non-uniform grids. Early discussions on discretization on non-uniform grids of self-adjoint (diffusive) equations can be found already in the work of Tikhonov and Samarskii [27] in the 1960’s; see also [22]. Somewhat later, Piacsek and Williams [19] explicitly advocated the use of a skew-symmetric analytic formulation in case of convective equations. Later, Veldman and Verstappen [28–30] showed that the same discretization can be obtained from the conservative divergence form of the equations. They subsequently extended this philosophy to fourth-order central discretization methods [31]. Closely related to this approach are the mimetic discretizations as developed by Steinberg and co-workers; see e.g. [23]. Also, the summation-by-parts property introduced by Strand [25] achieves similar properties of the discretization.

In the literature on (first-order) convective upwind methods, these properties have only occasionally been treated. An exception is e.g. [15], where upwind discretization is discussed in conjunction with the summation-by-parts property. The present paper applies the symmetry-preserving approach in an upwind vein. It is shown to lead to a variant for which the resulting coefficient matrix is always positive real, irrespective of grid (ir)regularity.

2. Discretization of the convection–diffusion equation

2.1. General concepts

In conservation form, the convection–diffusion equation reads

$$\int_{\Omega} \frac{\partial \phi}{\partial t} d\Omega + \int_{\Gamma} (\phi \vec{u} - k \text{grad } \phi) \cdot \vec{n} d\Gamma = 0, \quad (2)$$

for arbitrary domains Ω with boundary Γ . Here, the flow field $\vec{u} = (u, v)$ is assumed to satisfy $\text{div } \vec{u} = 0$ (incompressibility constraint), which in one dimension simplifies to $u = \text{constant}$. It is noted that analytically, ignoring influences from the boundaries, convection is a skew-symmetric operator, whereas diffusion is symmetric positive definite.¹ A discretization that mimics these analytical properties is called *symmetry preserving* [30,31] or *mimetic* [23].

The clue to the present note follows from Bendixson’s inclusion theorem as formulated e.g. by Householder [4, p. 69]:

All eigenvalues of a matrix A lie in or on the least rectangle with sides parallel to the real and imaginary axes that contains all eigenvalues of its symmetric and skew-symmetric part, respectively.

An immediate consequence is the following theorem:

Theorem 1. *Any symmetry-preserving discretization of the convection–diffusion equation (2) leads to a positive-real coefficient matrix. In particular, the latter matrix cannot become singular.*

¹ In order to prevent too much use of awkward phrases as ‘non-negative real’ or ‘non-negative definite’ it is assumed throughout this paper that diffusion operators have no eigenvalue equal to zero.

To understand the consequences of this theorem, consider the global error between the discrete solution ϕ_h and the analytical solution ϕ_{exact} . It is given by

$$\|\phi_h - \phi_{\text{exact}}\|_h = L^{-1}\tau,$$

where L is the discrete coefficient matrix and τ the local truncation error. Observe that the global error is built by the product of two factors: the local truncation error and the inverse coefficient matrix. Thus a ‘non-singular’ guarantee for L as given by Theorem 1 is highly relevant. Also, away from such a degenerate situation, the influence of the coefficient matrix appears quite important. This is observed for instance in extensive experiences with turbulent-flow simulations on structured [18,30,31] as well as unstructured grids [3].

2.2. Artificial diffusion

Consider a steady convection–diffusion equation in one space dimension (x), with a constant velocity u and with arbitrary $k = k(x) > 0$:

$$\frac{du\phi}{dx} - \frac{d}{dx} \left(k \frac{d\phi}{dx} \right) = 0, \quad x \in [0, 1], \quad (3)$$

provided with Dirichlet boundary conditions (for convenience) $\phi(0) = 0$, $\phi(1) = 1$. First-order upwind discretization of the convective term can be rewritten as a central discretization of the convective term $d(u\phi)/dx$ plus an artificial diffusion term, according to

$$\frac{du\phi}{dx} \rightarrow \frac{du\phi}{dx} - \frac{d}{dx} \left(\frac{1}{2}|u|h \frac{d\phi}{dx} \right) = \frac{d}{dx} \left(u - \frac{1}{2}|u|h \frac{d}{dx} \right) \phi. \quad (4)$$

Thus upwind discretization of (3) yields the same discrete equation as central discretization of

$$\frac{du\phi}{dx} - \frac{d}{dx} \left((k + k_{\text{art}}) \frac{d\phi}{dx} \right) = 0, \quad (5)$$

where $k_{\text{art}} := |u|h/2$ represents the artificial upwind diffusion.

2.3. A symmetry-preserving finite-volume upwind method

In this paper a conservative finite-volume approach is followed to achieve a symmetry-preserving discretization on arbitrary grids. Hereto, start with a non-uniform grid where the control faces are chosen halfway the grid points as in Fig. 1. In the one-dimensional version of (2), the flux function is given by

$$F(\phi) = u\phi - k \frac{d\phi}{dx}.$$

The convective and diffusive fluxes for (5) are chosen with second-order accuracy as (see notation in Fig. 1)

$$F(\phi)|_{i+1/2} := F(\phi_{i+1/2}) = u \frac{\phi_{i+1} + \phi_i}{2} - (k + k_{\text{art}})_{i+1/2} \frac{\phi_{i+1} - \phi_i}{h_+}. \quad (6)$$

The discrete unsteady convection–diffusion equation (2) then becomes

$$\frac{1}{2}(h_+ + h_-) \frac{d}{dt} \phi_i + \frac{1}{2}u(\phi_{i+1} - \phi_{i-1}) - (k + k_{\text{art}})_{i+1/2} \frac{\phi_{i+1} - \phi_i}{h_+} + (k + k_{\text{art}})_{i-1/2} \frac{\phi_i - \phi_{i-1}}{h_-} = 0. \quad (7)$$

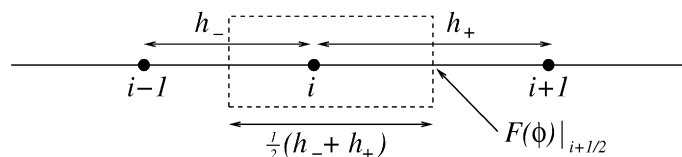


Fig. 1. One-dimensional control volume.

This expression falls in the framework from Section 1 with $H := \text{diag}\{\frac{1}{2}(h_+ + h_-)\}$, whereas the other coefficients in (7) form HL . The convective contribution is clearly skew symmetric, whereas the diffusive contribution is symmetric positive definite for any $k > 0$ and $k_{\text{art}} \geq 0$. Thus the matrix clearly satisfies the conditions in Theorem 1, and hence it is positive real for any non-negative choice of k_{art} .

In the upwind vain (4), it is natural to evaluate k_{art} using the ‘local’ value of the mesh size, i.e. to choose

$$(k_{\text{art}})_{i+1/2} := \frac{1}{2}|u|h_+. \quad (8)$$

By ‘reverse engineering’ the effective upwind discretization of the convective terms can be found. Combining the centrally discretized convective term in (7) with the k_{art} -part from the diffusive term results in

$$\frac{d\phi}{dx} \approx \frac{\phi_i - \phi_{i-1}}{\frac{1}{2}(h_+ + h_-)} = \frac{\phi_i - \phi_{i-1}}{\frac{1}{2}(x_{i+1} - x_{i-1})}. \quad (9)$$

This symmetry-preserving discretization is not obvious a priori. Because the denominator is not equal to the distance between the referred grid points, its local (pointwise) truncation error at first sight looks inconsistent on arbitrary grids: it is not exact for linear functions. Nevertheless, this discretization is also obtained by making an upwind choice for the convective flux function in (6): $F_{\text{conv}}(\phi)|_{i+1/2} := F_{\text{conv}}(\phi_i) = u\phi_i$. In a finite-volume context [7], the ‘inconsistency’ just mentioned is quite common, and is partly due to the interpretation of the discrete solution: does it represent grid point values or cell averages? There is no need to dwell on this issue here, however, as first-order pointwise accuracy can be proven anyway (see below).

As the above analysis reveals, discretization (9) guarantees that the coefficient matrix is always positive real. Moreover, inspection of (7) also reveals diagonal dominance, with non-positive entries outside the diagonal, i.e. it is an M -matrix [32]. Thus the following theorem has been obtained:

Theorem 2. *Upwind discretization of the one-dimensional convection–diffusion equation (3) by means of artificial diffusion according to $(k_{\text{art}})_{i+1/2} := |u|h_+/2$, generates a positive real M -matrix, irrespective of the grid.*

The non-uniformity of the grid makes the analysis of the global discretization error of (9) rather complicated, but it is still tractable. Manteuffel and White [14] have proven that, in absence of artificial diffusion, the symmetry-preserving central discretization given in (7) is second-order accurate on any (sufficiently fine) non-uniform grid (see also Hundsdorfer and Verwer [5, p. 271]). Their proof can be adapted to show that for artificial diffusion proportional to the local grid size, the solution of (7) is first-order accurate. More general considerations on convergence on irregular grids can be found in Kreiss et al. [10].

The symmetry-preserving discretization (9) is to be compared with the ‘traditional’ upwind discretization

$$\frac{d\phi}{dx} \approx \frac{\phi_i - \phi_{i-1}}{h_-} = \frac{\phi_i - \phi_{i-1}}{x_i - x_{i-1}}. \quad (10)$$

Because the effective local grid size in the denominator is now equal to the distance between the two grid points where ϕ is taken, approximation (10) is exact for linear functions. This method has theoretically been studied on non-uniform Bakhvalov and Shishkin grids by many authors, e.g. [9,11,13,17,20,21,26]. However, similar studies for the symmetry-preserving variant (9) are rare. Some information can be found in the recent overview by Linß [12] of upwind studies for layer-adapted non-uniform grids. These studies focus on theoretical asymptotic convergence rates, however no quantitative comparisons between the two approaches seem to have been made. Therefore, in Section 3.2 numerical experiments with both discretizations on (randomly generated) non-uniform grids will be presented.

2.4. Higher-order upwind

Higher-order upwind methods can also be built from skew-symmetric odd derivatives and positive-definite even derivatives. The following choice² gives a second-order accurate formulation (compare (4)):

² By changing the factor $1/2$ in front of the added term, symmetry-preserving variants of other schemes are formed, e.g. the value $1/8$ gives the QUICK method.

$$\frac{du\phi}{dx} \longrightarrow \frac{du\phi}{dx} - \frac{1}{2} \frac{d}{dx} \left(h \frac{d}{dx} \right) \left(u - \frac{1}{2} |u| h \frac{d}{dx} \right) \left(h \frac{d\phi}{dx} \right). \quad (11)$$

Analytically it is observed that the first- and third-order derivatives defined this way are skew-symmetric operators under the condition $\text{div } u = 0$, whereas the fourth-order derivative is always symmetric positive definite.

In one dimension (with $u > 0$) the second-order symmetry-preserving finite-volume discretization of the convective term thus becomes a familiar finite-volume approximation

$$\frac{d\phi}{dx} \approx \frac{3\phi_i - 4\phi_{i-1} + \phi_{i-2}}{x_{i+1} - x_{i-1}}. \quad (12)$$

Again, alternatives for the denominator exist such as $3x_i - 4x_{i-1} + x_{i-2}$, which makes the expression exact for linear functions. Also a Lagrangian interpolant can be fitted through the three discrete function values involved. However, none of these alternatives is symmetry preserving.

3. Numerical experiments

3.1. Eigenvalues of symmetric part

Golub et al. [1] gave the following example of a grid³ for which the traditional upwind discretization (10) is not positive real: $[0, 0.5, 0.51, 0.52, 1]$. Upwind discretization of (3) as in (10), for $u = 1$ and $k = 0.1$, leads to a scaled coefficient matrix $M_{\text{trad}} = 'HL'$ given by

$$M_{\text{trad}} = \begin{pmatrix} 10.7 & -10.0 & 0.0 \\ -11.0 & 21.0 & -10.0 \\ 0.0 & -34.5 & 34.7 \end{pmatrix}$$

(note that our scaling H differs a factor of two from the one used by Golub et al.; also u has been normalized). Its eigenvalues (λ) and those of its symmetric part, denoted by $M_{\text{trad}}^{\text{sym}}$, are given by

$$\lambda(M_{\text{trad}}) = \{0.35, 17.42, 48.65\} \quad \text{and} \quad \lambda(M_{\text{trad}}^{\text{sym}}) = \{-1.60, 15.90, 52.11\},$$

revealing one negative eigenvalue of the symmetric part. Golub et al. [1] argue that the non-monotonicity of the grid (the grid size is contracting and expanding in the flow direction) is responsible for this behavior; we will give more evidence below.

On the other hand, upwind discretization in the symmetry-preserving vein according to (9) leads to the coefficient matrix (note the large difference with the above matrix in the ‘expanding’ grid point)

$$M_{\text{s-p}} = \begin{pmatrix} 11.2 & -10.0 & 0.0 \\ -11.0 & 21.0 & -10.0 \\ 0.0 & -11.0 & 11.2 \end{pmatrix}.$$

Its eigenvalues and those of its symmetric part are given by

$$\lambda(M_{\text{s-p}}) = \{0.48, 11.2, 31.72\} \quad \text{and} \quad \lambda(M_{\text{s-p}}^{\text{sym}}) = \{0.47, 11.20, 31.74\}.$$

Indeed, as implied by Theorem 2, all eigenvalues of the symmetric part are positive now.

The differences between the two discretizations can be made larger when moving the clustered grid points closer together. Let us generalize the above grid to

$$x_i := [0, 0.5, 0.5 + \delta, 0.5 + 2\delta, 1]. \quad (13)$$

Table 1 shows the behavior of the extremal ‘upwind’ eigenvalues as a function of δ and k (smaller values of k are more interesting from an upwind point of view). It is observed that, for smaller values of δ , not only the eigenvalues of the symmetric part are moving away in both directions, but also the right-most eigenvalue of the ‘traditional’ coefficient matrix itself is moving away from the axis. This limits the stability time step for explicit time-integration methods. In the symmetry-preserving method this effect is reduced for smaller k ; see also the discussion in Section 3.3.

³ One small grid cell would have sufficed to demonstrate the phenomenon, but we prefer to stick to their original example.

Table 1

Upwind eigenvalues on grids with clustered grid points (13), for the traditional upwind discretization (10) and the symmetry-preserving variant (9)

k	δ	'traditional' upwind				symm.-pres. upwind			
		$\lambda(M_{\text{trad}})$		$\lambda(M_{\text{trad}}^{\text{sym}})$		$\lambda(M_{\text{s-p}})$		$\lambda(M_{\text{s-p}}^{\text{sym}})$	
		min	max	min	max	min	max	min	max
10^{-1}	10^{-2}	0.35	48.65	−1.60	52.11	0.48	31.72	0.47	31.74
10^{-1}	10^{-4}	0.33	4850.9	−200.3	5205.8	0.47	3001.7	0.47	3001.7
10^{-3}	10^{-2}	0.44	24.71	−4.18	29.92	0.68	1.62	0.30	2.00
10^{-3}	10^{-4}	0.26	2519.6	−505.6	3035.9	0.35	31.65	0.33	31.67
10^{-5}	10^{-2}	0.51	24.50	−4.27	29.73	0.96	1.05	0.29	1.71
10^{-5}	10^{-4}	0.43	2499.7	−516.7	3017.5	0.68	1.62	0.30	2.00

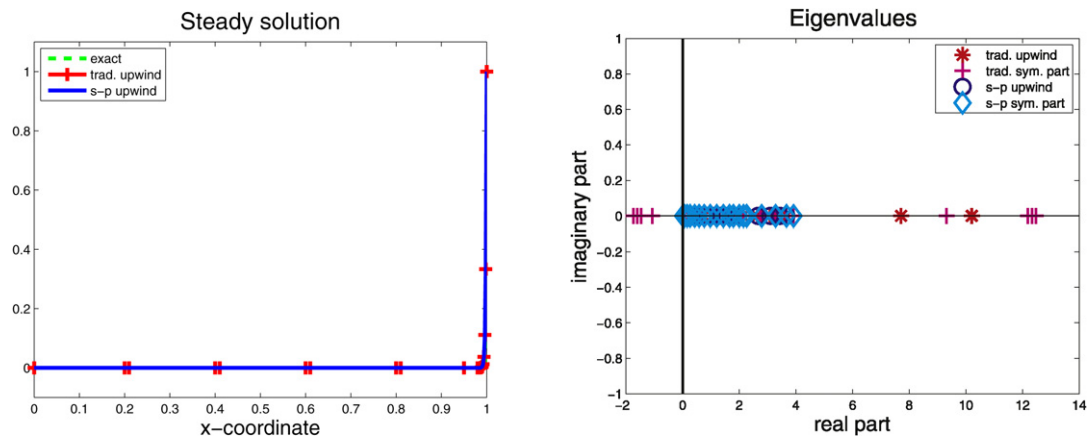


Fig. 2. Eigenvalues of the upwind variants on a grid with four clusters (14). Left: the discrete solutions; the grid points are also visible. Right: the 'rebellious' eigenvalues on both sides of the spectrum for the traditional upwind method are clearly visible.

Until here, we have used the flow parameters chosen by Golub et al. [1]; from now on we set $u = 1$ and $k = 0.001$. As another illustrative example we take a grid with four clustered pairs of grid points, combined with a reasonable resolution of the boundary layer:

$$x_i := [0, 0.2, 0.21, 0.4, 0.41, 0.6, 0.61, 0.8, 0.81, 0.95, 0.98 : 0.002 : 1.0]. \quad (14)$$

It is found that now four eigenvalues of the symmetric part are negative (Fig. 2). By experimenting with similar grids, there appears to be a relation between the distribution of the eigenvalues (how many eigenvalues are moving away) and the (number of) contractive grid-point clusters; however, we will not elaborate on this issue here.

For non-monotone grids with contraction and expansion in the flow direction, as considered here, it is not too difficult to create the above phenomena, as the examples show. For the one-dimensional case discussed here, such grids are rather illogical. But in more dimensions, non-monotone regions in the grid cannot always be avoided, because of grid constraints elsewhere in the flow domain.

Also, with the second-order upwind discretization from Section 2.4 some experiments have been carried out (near the boundary $x = 0$, the 'missing' discrete value outside the interval has been set to its exact value). The same observations as with first-order upwind discretization have been made. Golub's example again shows one negative eigenvalue of the symmetric part when the traditional Lagrangian discretization is followed: the spectrum becomes $\{-4.75, 10.87, 72.82\}$. In comparison, the spectrum of the symmetric part of the symmetry-preserving variant (12) is $\{0.46, 11.45, 33.00\}$. Further, the four-cluster grid (14) generates again four negative eigenvalues of the 'traditional' symmetric part. Thus, second-order upwind discretization shows the same phenomena with respect to the positioning of the eigenvalues of the coefficient matrix as first-order upwind discretization.

3.2. Convergence analysis

The local truncation error of the symmetry-preserving discretization method (9) at first sight does not look promising. However, in a finite-volume setting the non-exactness for linear solutions is familiar in cell-centered methods, and our concern need not be too large. Indeed, this section will show that the method behaves first order, as theoretically predicted in Section 2.3. Hereto, first calculations on a stretched Shishkin grid will be carried out. Originally, this is a grid consisting of two uniform subintervals separated by the point $x = x_s := \max(0.5, 1 - k \ln N)$, where N is the total number of grid points; see e.g. Hemker et al. [2]. Each of the two subintervals contains half of the grid points. For the ‘traditional’ upwind method on such a grid k -uniform convergence has been proven [17]. With minor changes, this proof also holds for the symmetry-preserving upwind variant.

A Shishkin grid contains only one ‘non-uniform’ grid point, hence little difference is expected between both methods. More differences are expected on an exponentially stretched grid, obtained from the transformation

$$x = x(\xi) := \frac{1 - c^\xi}{1 - c} \quad (\xi \in [0, 1]) \text{ with } c = \frac{1 - x_s}{x_s},$$

where c has been chosen such that $\xi = 0.5$ corresponds with the split point x_s of the Shishkin grid. The global error $\|\phi_h - \phi_{\text{exact}}\|_h$ has been monitored; results are shown in Fig. 3 (left). A (close to) first-order convergence is visible for both methods, with the symmetry-preserving method being more accurate.

We also have studied random grids, generated in ξ from a uniform random distribution on the interval $[0, 1]$. Thus, on average both ‘Shishkin’ intervals contain the same number of grid points. In this way some variation is brought in the expansion and contraction of the grid, whereas still there is (reasonable) resolution in the boundary layer. A series of 89 grids has been selected, with the number of grid points increasing from 11 to 99. Fig. 3 (right) shows the global error as a function of the number of grid points for both upwind approaches. A least-squares fit reveals a (more or less) first-order convergence behavior for both methods, whereas for almost each individual grid the symmetry-preserving variant appears to produce a smaller global error. This in spite of the fact that the local truncation error of (9) on arbitrary grids looks worse than that of (10). As indicated already in Section 2.1, the matrix properties turn out to be more important than (formal) local truncation error.

Also, some experiments with second-order upwind methods have been carried out. A comparison between the results of Lagrangian interpolation and the symmetry-preserving discretization (12) on an exponential Shishkin grid is presented in Fig. 4. Again, as in Fig. 3, the symmetry-preserving variant is found more accurate than its ‘traditional’ counterpart.

3.3. Right-most eigenvalue

As already demonstrated above, also the right-most eigenvalue of the coefficient matrix is influenced by the expanding character of the grid. This eigenvalue controls the diffusive stability limit of explicit time integration methods.

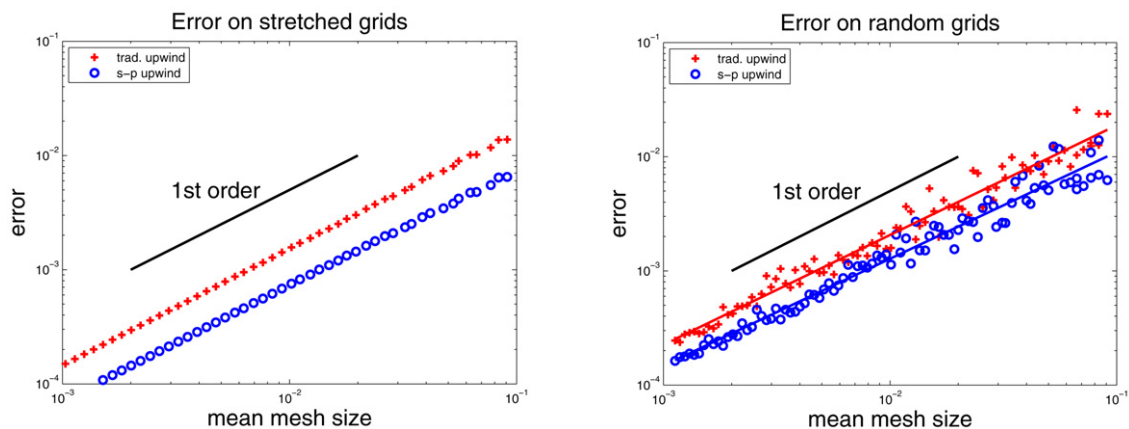


Fig. 3. Grid refinement for the ‘traditional’ upwind discretization (10), and the symmetry-preserving variant (9). Left: exponentially stretched grids; right: stretched random grids.

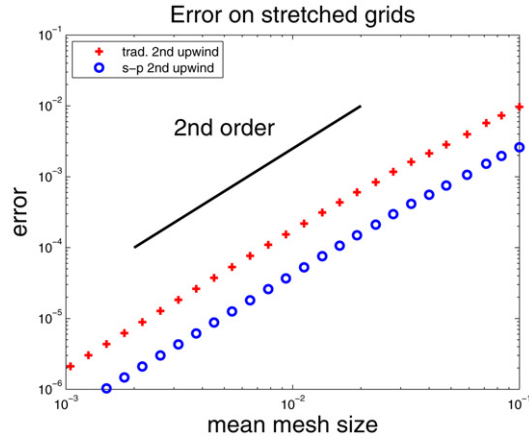


Fig. 4. Symmetry-preserving second-order upwind discretization (12) on exponentially stretched grids compared with its second-order Lagrangian counterpart.

In the above (extreme grid) example it moves towards the origin when the symmetry-preserving upwind discretization (9) is used, thus enhancing explicit stability. This influence can be understood from a theoretical analysis, as shown next.

In the limit of vanishing diffusion, the position of the right-most eigenvalue for the first-order discretization (9) can easily be investigated by analytical means. On a grid $[x_i]_{i=0,\dots,N}$, the eigenvalues of the matrices M_{trad} and $M_{\text{s-p}}$ are given by

$$\lim_{k \rightarrow 0} \lambda(M_{\text{trad}}) = \frac{u}{2} \left(1 + \frac{x_{i+1} - x_i}{x_i - x_{i-1}} \right) \quad (i = 1, \dots, N-1); \quad (15)$$

$$\lim_{k \rightarrow 0} \lambda(M_{\text{s-p}}) = u \quad ((N-1)\text{-fold}). \quad (16)$$

Indeed, when the grid size is increasing in flow direction, i.e. $x_{i+1} - x_i > x_i - x_{i-1}$, the eigenvalues of $\lim_{k \rightarrow 0} M_{\text{trad}}$ can become arbitrarily large, whereas the eigenvalues of $\lim_{k \rightarrow 0} M_{\text{s-p}}$ are not affected by the grid. This tendency is clearly visible in Table 1. On the grid (13) for small k , (15) at $i = N-1$ predicts largest eigenvalues of 24.5 at $\delta = 10^{-2}$ and 2499.5 at $\delta = 10^{-4}$; the smallest eigenvalue is predicted at $i = 1$ to be ≈ 0.5 . These values are quite close to the $k = 10^{-5}$ -values in Table 1. On the other hand, the symmetry-preserving expression (16) predicts (much smaller) eigenvalues approaching ($u =$) 1, which also is in line with the numerically found values.

Similar expressions hold for the eigenvalues of the non-scaled matrix $L = H^{-1}M$, which controls the time step of explicit time integration. Again, the eigenvalues of $\lim_{k \rightarrow 0} L_{\text{trad}}$ can be arbitrarily larger than those of $\lim_{k \rightarrow 0} L_{\text{s-p}}$. This difference in the position of the extremal eigenvalues makes explicit time integration with the traditional upwind discretization (10) more expensive on grids that expand in flow direction.

4. More space dimensions – unstructured first-order

In two (or more) dimensions, the velocity field $\vec{u} = (u, v)$ is allowed to vary over the domain of interest, as long as \vec{u} is divergence free, i.e. $\text{div } \vec{u} = 0$. Thus, the consequences of a non-constant velocity field become visible. The above first-order upwind discretization (9) is easily generalized to unstructured grids.

Consider part of an unstructured grid as in Fig. 5, with a central grid point O and neighboring grid points A, B, \dots, F . The control volume around O is chosen according to a Voronoi tessellation, i.e. the cell faces are the perpendicular bisectors of the lines connecting the grid points, as advocated for instance in [33] (note that this differs from the more usual centroid-based control volumes [16]). A straightforward discretization of (2) yields in first instance

$$\delta s_a \left(q_a \phi_a - k_a \frac{\partial \phi}{\partial n} \Big|_a \right) + \delta s_b \left(q_b \phi_b - k_b \frac{\partial \phi}{\partial n} \Big|_b \right) + \dots + \delta s_f \left(q_f \phi_f - k_f \frac{\partial \phi}{\partial n} \Big|_f \right) = 0.$$

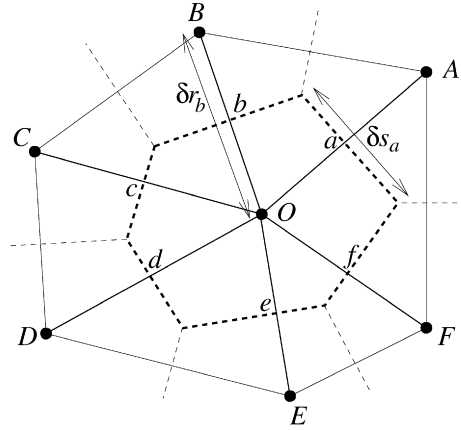


Fig. 5. Two-dimensional control volume: Voronoi tessellation.

Here δs is the length of a cell face, n is the outward-pointing normal, and q is the velocity component in normal direction.

As the points a, b, \dots, f lie half-way the grid points, the fluxes through the faces of the control volume are found with second-order accuracy, leading to

$$\begin{aligned} \delta s_a \left(q_a \frac{\phi_A + \phi_O}{2} - k_a \frac{\phi_A - \phi_O}{\delta r_a} \right) + \delta s_b \left(q_b \frac{\phi_B + \phi_O}{2} - k_b \frac{\phi_B - \phi_O}{\delta r_b} \right) + \dots \\ + \delta s_f \left(q_f \frac{\phi_F + \phi_O}{2} - k_f \frac{\phi_F - \phi_O}{\delta r_f} \right) = 0. \end{aligned} \quad (17)$$

If the continuity equation $\text{div } \vec{u} = 0$ has been discretized with the same control volume, then

$$\delta s_a q_a + \delta s_b q_b + \dots + \delta s_f q_f = 0. \quad (18)$$

Combining this with (17), it is observed that the contribution from ϕ_O to the convective term vanishes! The following discrete equation results

$$\begin{aligned} \delta s_a \left(\frac{q_a}{2} - \frac{k_a}{\delta r_a} \right) \phi_A + \delta s_b \left(\frac{q_b}{2} - \frac{k_b}{\delta r_b} \right) \phi_B + \dots + \delta s_f \left(\frac{q_f}{2} - \frac{k_f}{\delta r_f} \right) \phi_F \\ + \left(\frac{\delta s_a}{\delta r_a} k_a + \frac{\delta s_b}{\delta r_b} k_b + \dots + \frac{\delta s_f}{\delta r_f} k_f \right) \phi_O = 0. \end{aligned} \quad (19)$$

The upwind discretization follows by adding the artificial diffusion to the natural diffusion, i.e. replace $k \rightarrow k + k_{\text{art}}$, as in [7,6]. Again the local value for k_{art} should be used, e.g. $(k_{\text{art}})_a := |q_a| \delta r_a / 2$. Spalding [24] argued that the amount of upwind diffusion necessary to obtain an M -matrix is smaller than given by (8), because the physical diffusion is available. His choice for the artificial diffusion amounts to the replacement $k \rightarrow \max\{k, k_{\text{art}}\}$. As k_{art} vanishes for sufficiently small grid size, this method (obviously) becomes second-order, although on coarse grids it is very comparable to first-order upwind. Linß [12] analyses this choice at length in the context of Bakhvalov and Shishkin grids (although at a different effective local grid size, cf. the discussion above on the difference between (10) and (9)).

Now we are able to formulate our concluding theorem, the proof of which is fairly straightforward.

Theorem 3. *When the discrete velocity field is divergence free (18), then for any (non-negative) artificial diffusion, the conservative discretization (17) is symmetry-preserving and hence positive real. Moreover, when upwind discretization is generated by adding artificial diffusion to (19) according to*

$$(k_{\text{art}})_a \geq \max \left\{ \frac{1}{2} |q_a| \delta r_a - k_a, 0 \right\}, \quad \text{etc.}, \quad (20)$$

then the coefficient matrix of (19) is a diagonally dominant, positive real M -matrix.

5. Discussion

Several ways exist to implement an upwind discretization of convection. Golub et al. [1] have shown that the ‘traditional’ way of constructing a one-sided discretization (10) does not always lead to a positive real coefficient matrix, in particular on grids that contract and expand in the direction of the flow. On the other hand, the present note proves that (conservative) upwind discretization (9) implemented in a symmetry-preserving way, i.e. as a central discretization plus artificial diffusion, does always lead to a diagonally-dominant positive real matrix, irrespective of the underlying computational grid. Also, on (randomly) stretched grids it is found that the symmetry-preserving upwind method usually is more accurate than the ‘traditional’ upwind method. Moreover, on Shishkin grids k -uniform convergence can be proven. Furthermore, the location of the extremal eigenvalues in many cases is found to be more favorable. Finally, the implementation costs of both approaches are similar.

The subtle difference between the two formulations seems not to have been stressed in the literature. Most theoretical work on upwind methods for Shishkin grids is restricted to the ‘traditional’ approach [12]. The more ‘practical’ finite-volume community uses the other formulation, following [7]. However, no direct performance comparison between the two approaches seems to have been made.

The present paper intends to contribute to such a direct comparison. The numerical experiments presented show that, as for its higher-order counterparts [31], the symmetry-preserving and conservative upwind method appears quite forgiving with respect to grid irregularity and grid coarseness; even more so than the traditional upwind formulation. In this respect, the symmetry-preserving upwind variant is a good candidate to replace traditional upwind discretization in underresolved flow calculations. It would be interesting to develop more theory behind the observations, especially with respect to the coarse-grid behavior, such that this recommendation can be founded better.

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